21st Century High-End Computing

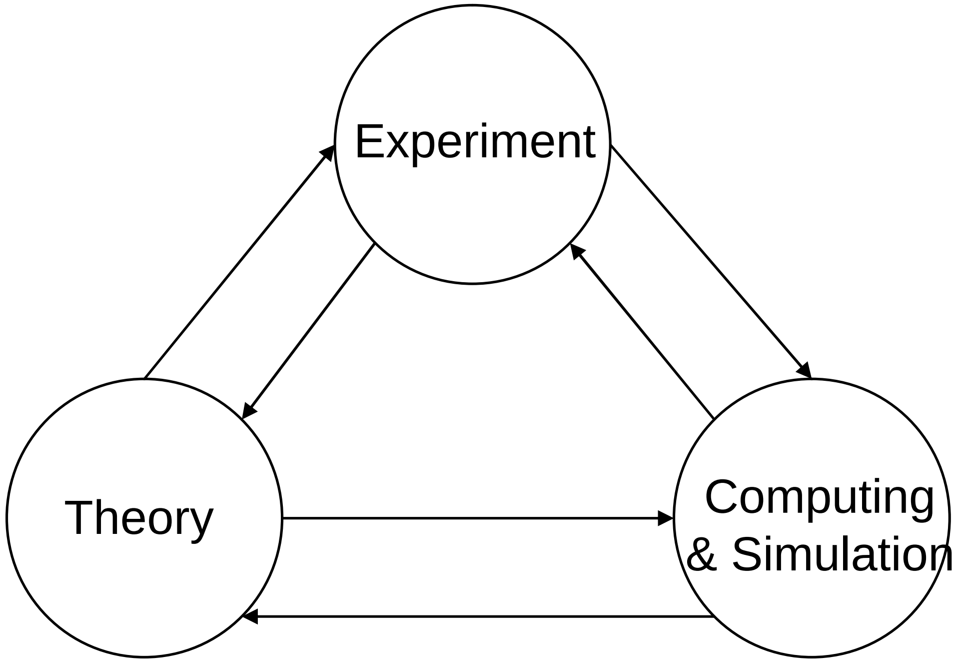
David H. Bailey
Chief Technologist, NERSC
Lawrence Berkeley National Laboratory
http://www.nersc.gov/~dhbailey

Laplace Anticipates Modern High-End Computers

"An intelligence knowing all the forces acting in nature at a given instant, as well as the momentary positions of all things in the universe, would be able to comprehend in one single formula the motions of the largest bodies as well as of the lightest atoms in the world, provided that its intellect were sufficiently powerful to subject all data to analysis; to it nothing would be uncertain, the future as well as the past would be present to its eyes."

-- Pierre Simon Laplace, 1773

Computing as the Third Mode of Discovery



Numerical simulations: experiment by computation.

Who Needs High-End Computers?

Expert predictions:

- (c. 1945) Thomas J. Watson (CEO of IBM):
  "World market for maybe five computers."
- (c. 1975) Seymour Cray:
  "Only about 100 potential customers for Cray-1."
- *(c. 1977) Ken Olson (CEO of DEC):*
  "No reason for anyone to have a computer at home."
- (c. 1980) IBM study:
  "Only about 50 Cray-1 class computers will be sold per year."

Present reality:

- Many homes now have 5 Cray-1 class computers.
- Latest PCs outperform 1988-era Cray-2.

Evolution of High-End Computing Technology

1950	Univac-1	1 Kflop/s (10^3 flop/sec)
1965	IBM 7090	100 Kflop/s (10^5 flop/sec)
1970	CDC 7600	10 Mflop/s (10^7 flop/sec)
1976	Cray-1	100 Mflop/s (10^8 flop/sec)
1982	Cray X-MP	1 Gflop/s (10^9 flop/sec)
1990	TMC CM-2	10 Gflop/s (10^{10} flop/sec)
1995	Cray T3E	100 Gflop/s (10^{11} flop/sec)
2000	IBM SP	1 Tflop/s (10^{12} flop/sec)
2002	Earth Simulator	40 Tflop/s (4×10^{12} flop/sec)

Evolution of High-End Scientific Applications

- Infeasible – much too expensive to consider.
- First sketch of possible computation.
- First demo on state-of-the-art high-end system.
- Code is adapted by other high-end researchers.
- Code runs on single-node shared memory system.
- Code runs on single-CPU workstation.
- Production and engineering versions appear.
- Code runs on personal computer system.
- Code is embedded in browser.
- Code is available in hand-held device.

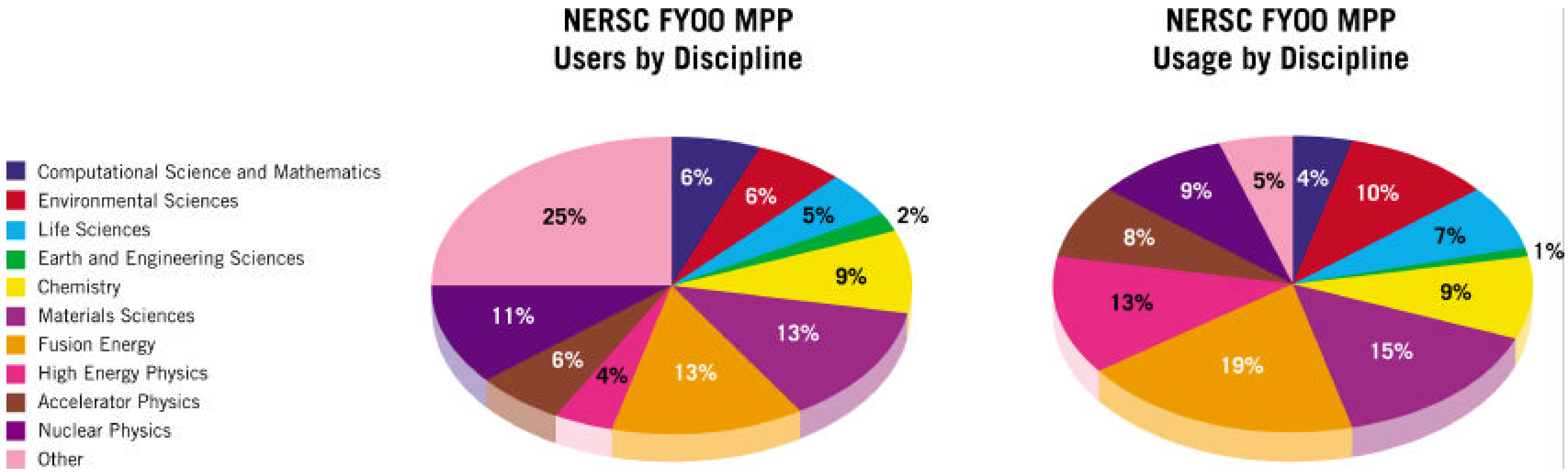
NERSC, LBNL and DOE

- The National Energy Research Scientific Computing Center (NERSC) moved to the Berkeley Lab in 1996.
- Provides state-of-the-art supercomputer resources to researchers throughout the U.S. working on science projects funded through the U.S. Dept. of Energy.

NERSC-3 (Seaborg) System

- 3328-CPU IBM SP: 5 Tflop/s (5 trillion flops/sec).
- Currently the world's 3rd most powerful computer.

The NERSC User Community

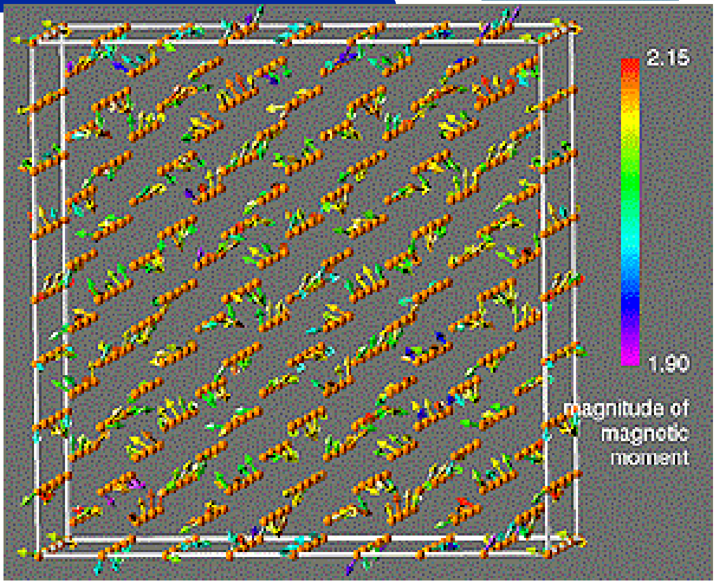


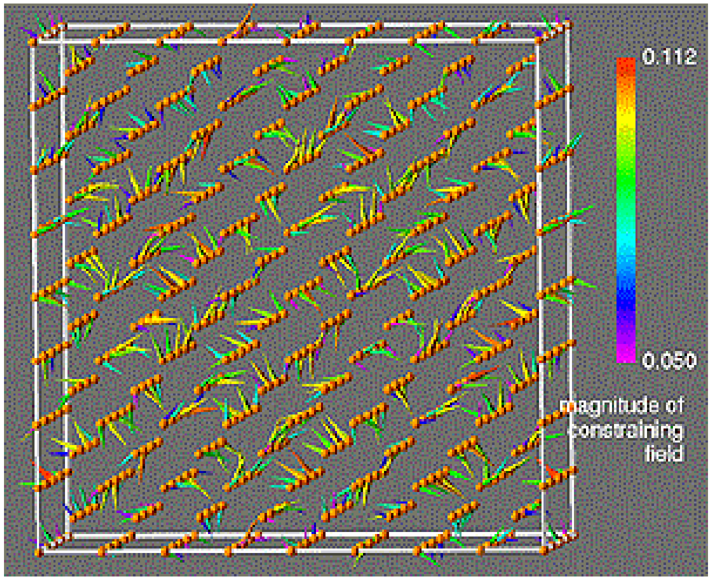
NERSC/DOE Applications: Materials Science

1024-atom first-principles simulation of metallic magnetism in iron.

• 1998 Gordon Bell Prize winner -- first real scientific simulation to run faster than 1Tflop/s.

• New 2016-atom simulation now runs on the NERSC-3 system at 2.46 Tflop/s.



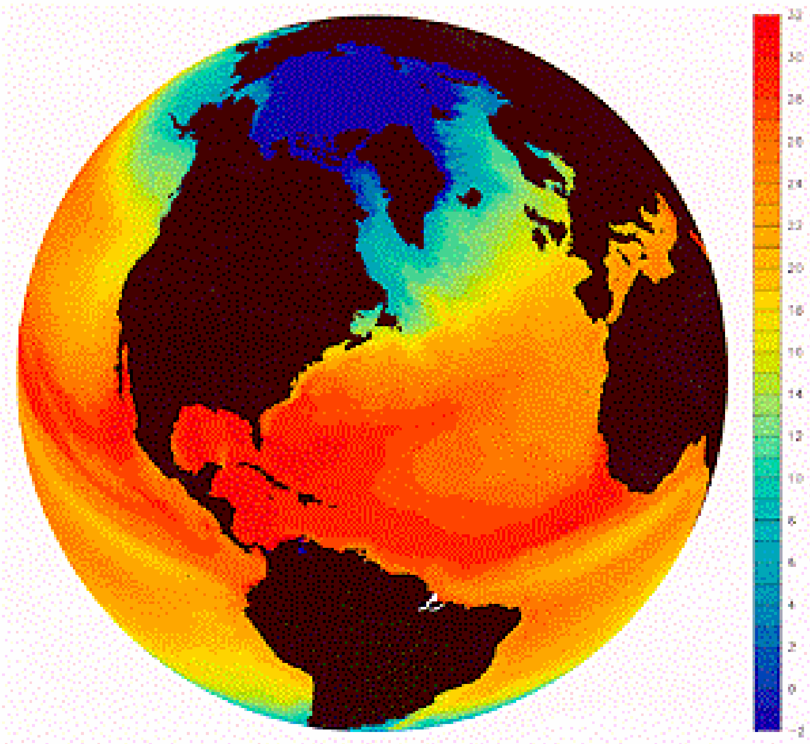


Materials Science Requirements

- Electronic structures:
  - Current: ~300 atom: 0.5 Tflop/s, 100 Gbyte memory.
  - Future: ~3000 atom: 50 Tflop/s, 2 Tbyte memory.
- Magnetic materials:
  - Current: ~2000 atom: 2.64 Tflop/s, 512 Gbytes memory.
  - Future: hard drive simulation: 30 Tflop/s, 2 Tbyte memory.
- Molecular dynamics:
  - Current: 10^9 atoms, ns time scale: 1 Tflop/s, 50 Gbyte mem.
  - Future: alloys, us time scale: 20 Tflop/s, 4 Tbyte memory.
- Continuum solutions:
  - Current: single-scale simulation: 30 million finite elements.
  - Future: multiscale simulations: 10 x current requirements.

NERSC/DOE Applications: Environmental Science

Parallel climate model (PCM) simulates long-term global warming.

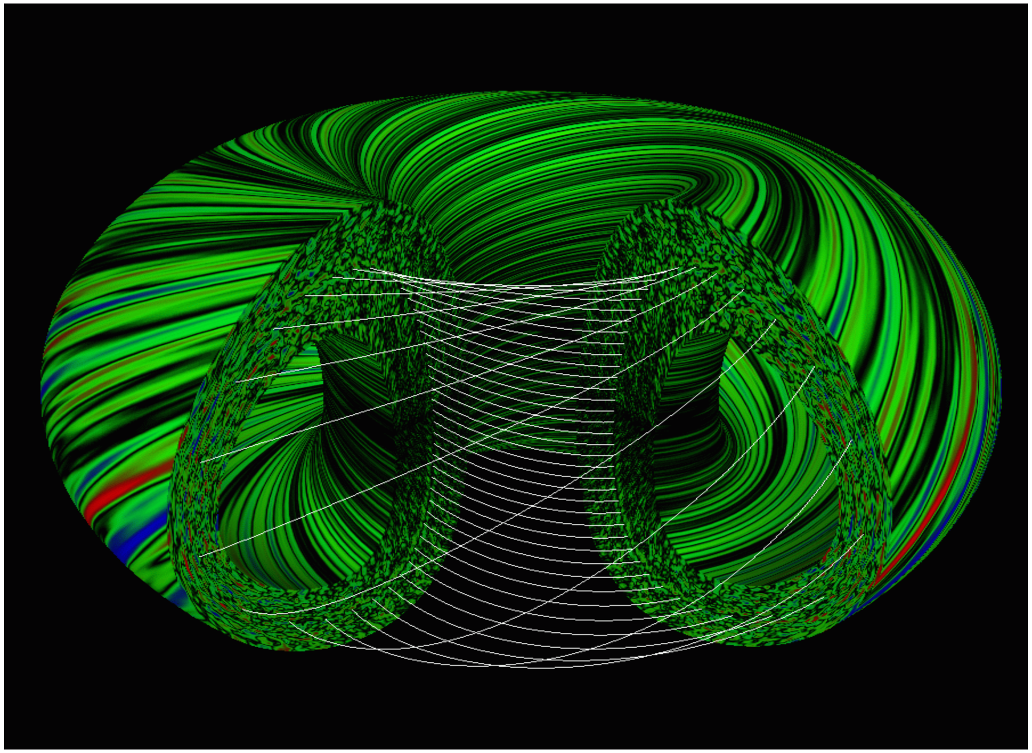


Climate Modeling Requirements

- Current state-of-the-art:
  - Atmosphere: 1 x 1.25 deg spacing, with 29 vertical layers.
  - Ocean: 0.25 x 0.25 degree spacing, 60 vertical layers.
  - Currently requires 52 seconds CPU time per simulated day.
- Future requirements (to resolve ocean mesoscale eddies):
  - Atmosphere: 0.5 x 0.5 deg spacing.
  - Ocean: 0.125 x 0.125 deg spacing.
  - Computational requirement: 17 Tflop/s.
- Future goal: resolve tropical cumulus clouds:
  - 2 to 3 orders of magnitude more than above.

NERSC/DOE Applications: Fusion Energy

Computational simulations help scientists understand turbulent plasmas in nuclear fusion reactor designs.

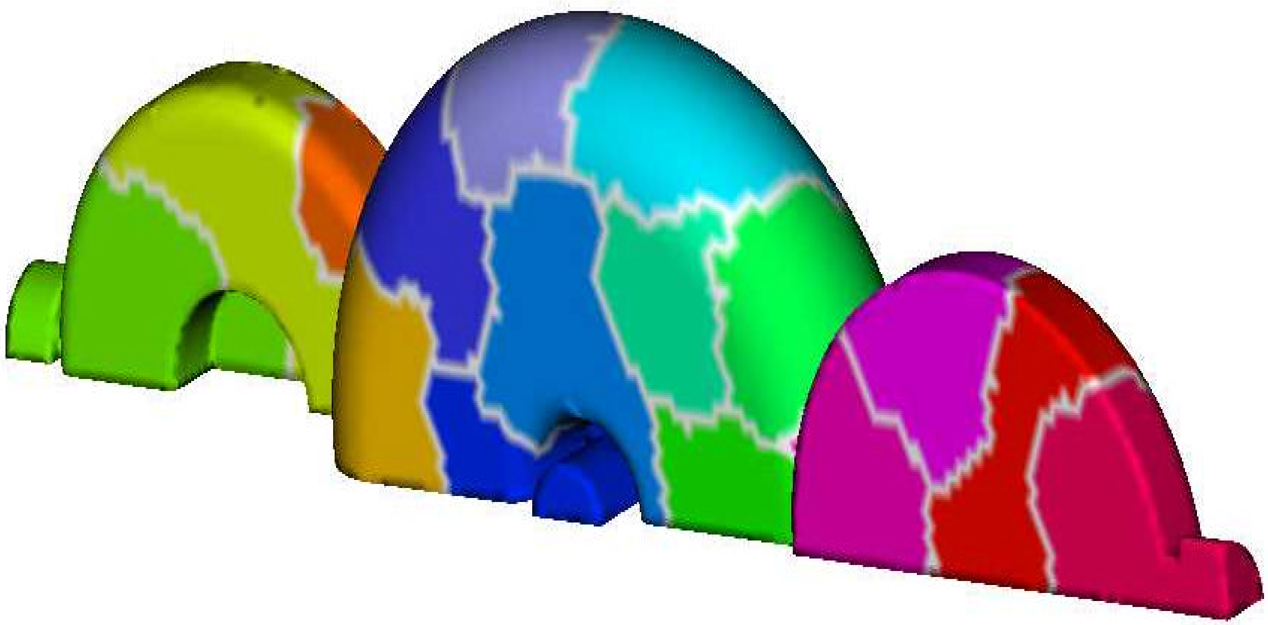


Fusion Requriements

- Tokamak simulation -- ion temperature gradient turbulence in ignition experiment:
  - Grid size: 3000 x 1000 x 64, or about 2 x 10^8 gridpoints.
  - Each grid cell contains 8 particles, for total of 1.6 x 10^9.
  - 50,000 time steps required.
  - Total cost: 3.2 x 10^{17} flop/s, 1.6 Tbyte.
- All-Orders Spectral Algorithm (AORSA) – to address effects of RF electromagnetic waves in plasmas.
  - 120,000 x120,000 complex linear system.
  - 230 Gbyte memory.
  - 1.3 hours on 1 Tflop/s.
  - 300,000 x 300,000 linear system requires 8 hours.
  - Future: 6,000,000 x 6,000,000 system (576 Tbyte memory), 160 hours on 1 Pflop/s system.

NERSC/DOE Applications: Accelerator Physics

Simulations are being used to design future high-energy physics research facilities.

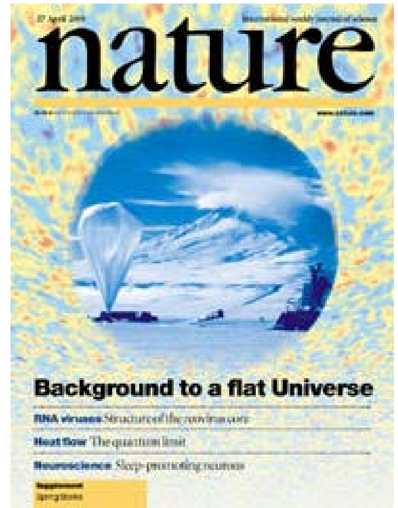


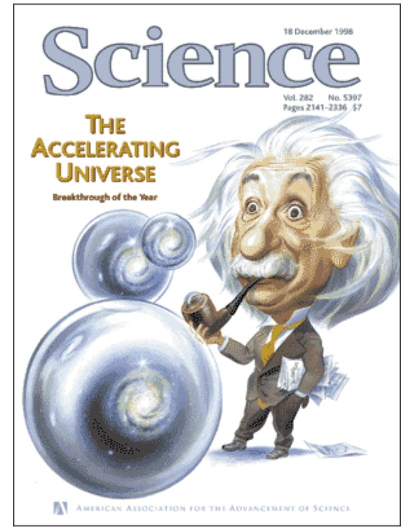
Accelerator Modeling Requirements

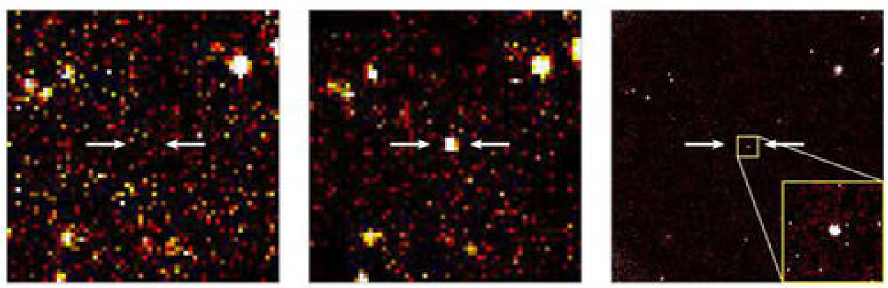
- Current computations:
  - 1283 to 5123 cells, or 40 million to 2 billion particles.
  - Currently requires 10 hours on 256 CPUs.
- Future computations:
  - Modeling intense beams in rings will be 100 to 1000 times more challenging.

NERSC/DOE Applications: Astrophysics and Cosmology

- The oldest, most distant Type 1a supernova confirmed by computer analysis at NERSC.
- Supernova results point to an accelerating universe.
- Analysis at NERSC of cosmic microwave background data shapes concludes that geometry of the universe is flat.





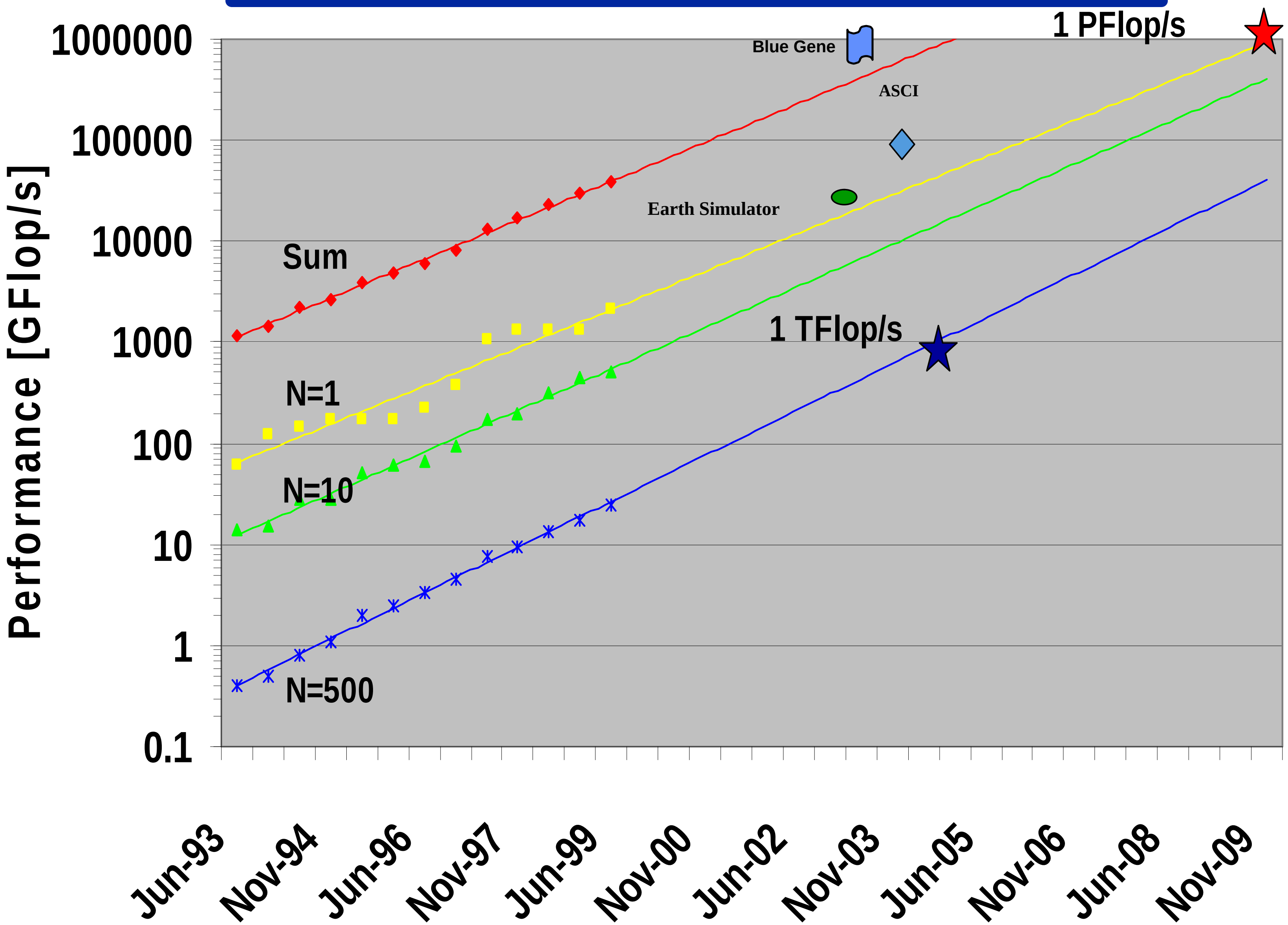


Astrophysics Requirements

- Supernova simulation:
  - Critical need to better understand Type Ia supernovas, since these are used as “standard candles” in calculating distances to remote galaxies.
  - Current models are only 2-D.
  - Initial 3-D model calculations will require 2,000,000 CPU-hours per year, on jobs exceeding 256 Gbyte memory.
  - Future calculations 10 to 100 times as expensive.
- Analysis of cosmic microwave background data:

MAXIMA data	5.3×10^{16} flops	100 Gbyte mem
BOOMERANG data	1.0×10^{19} flops	3.2 Tbyte mem
Future MAP data	1.0×10^{20} flops	16 Tbyte mem
Future PLANCK data	1.0×10^{23} flops	1.6 Pbyte mem

Top500 Trends



Top500 Data Projections

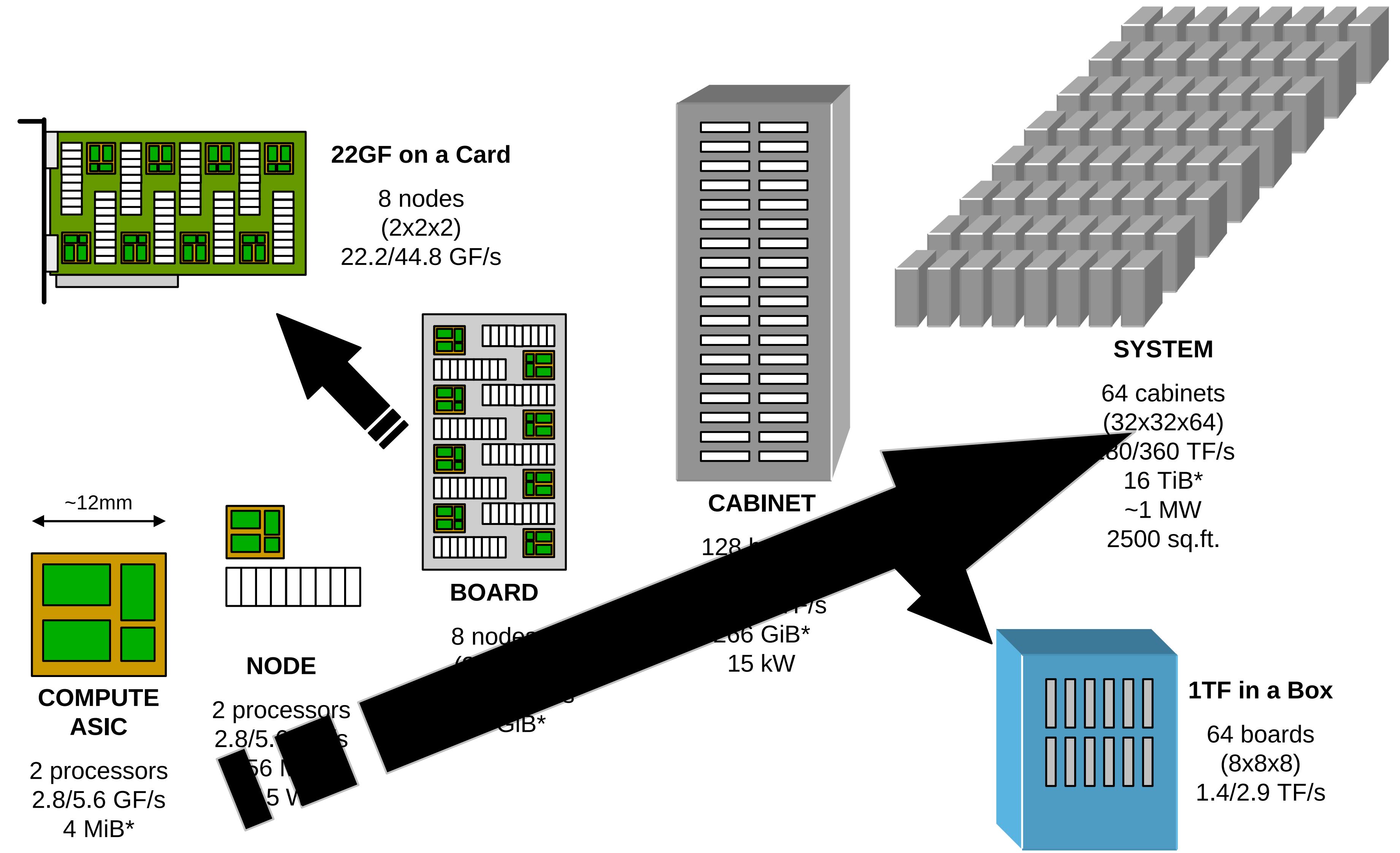
- First 100 Tflop/s system by 2005.
- No system under 1 TFlop/s will make the Top500 list by 2005.
- First commercial Pflop/s system will be available in 2010.

For info on Top500 list, see http://www.top500.org

The Japanese Earth Simulator System

- System design:
  - Performance: 640 nodes x 8 proc per node x 8 Gflop/s per proc = 40.96 Tflop/s peak.
  - Memory: 640 nodes x 16 Gbyte per node = 10.24 Tbyte.
- Sustained performance:
  - Global atmospheric simulation: 26.6 Tflop/s.
  - Fusion simulation (all HPF code): 12.5 Tflop/s.
  - Turbulence simulation (global FFTs): 12.4 Tflop/s.

IBM's Blue Gene/L Project Design Points



UCRL-PRES-146991

Other Future High-End Designs

- Processor in memory
  - Currently being pursued by a team headed by Prof. Thomas Sterling of Cal Tech.
  - Seeks to design a high-end scientific system based on special processors with embedded memory.
  - Advantage: significantly greater processor-memory bandwidth.
- Streaming supercomputer
  - Currently being pursued by a team headed by Prof. William Dally of Stanford.
  - Seeks to adapt streaming processing technology, now used in game market, to scientific computing.
  - Projects 200 Tflop/s, 200 Tbyte system will cost $10M in 2007.

Petaflops Computing

- 1 Pflop/s (10^{15} flop/sec) in computing power.
- Between 10,000 and 100,000 individual CPUs.
- Between 10 Tbyte and 1 Pbyte main memory (= 100x the UC Berkeley library).
- Between 10 and 100 Pbyte on-line mass storage.
- If built today, a petaflops system would cost $1 billion and consume 100 Mwatts of electric power.
- Programming challenge: 10^8-way concurrency at all significant steps of a computation.

Future Applications for Petaflops Systems

- Weather forecasting.
- Business data mining.
- DNA sequence analysis.
- Protein folding simulations.
- Nuclear weapons stewardship.
- Multiuser immersive virtual reality.
- National-scale economic modeling.
- Climate and environmental modeling.
- Symbolic and experimental mathematics.
- Cryptography and digital signal processing.
- Design tools for molecular nanotechnology.

Moore’s Law Beyond 2010

- At or about the year 2010, semiconductor technology will reach the “0.1 micron” barrier.
- Possible solutions:
  - A mirror-based extreme ultraviolet system – under development by researchers at Intel and government labs, including LBNL.
  - X-rays or electron beams.
  - Atomic force microscope “combs.”

One way or another, Moore’s Law almost certainly will continue beyond 2010, maybe beyond 2020.

Fundamental Limits of Devices

Assume a power dissipation of 1 watt at room temperature, and 1 cm^3 volume.

- How many bit operation/second can be performed by a nonreversible computer executing Boolean logic?
  - Ans: P/kT log(2) = 3.5×10^{20} bit ops/s
- How many bits/second can be transferred?
  - Ans: sqrt(cP/kTd) = 10^{18} bit/s

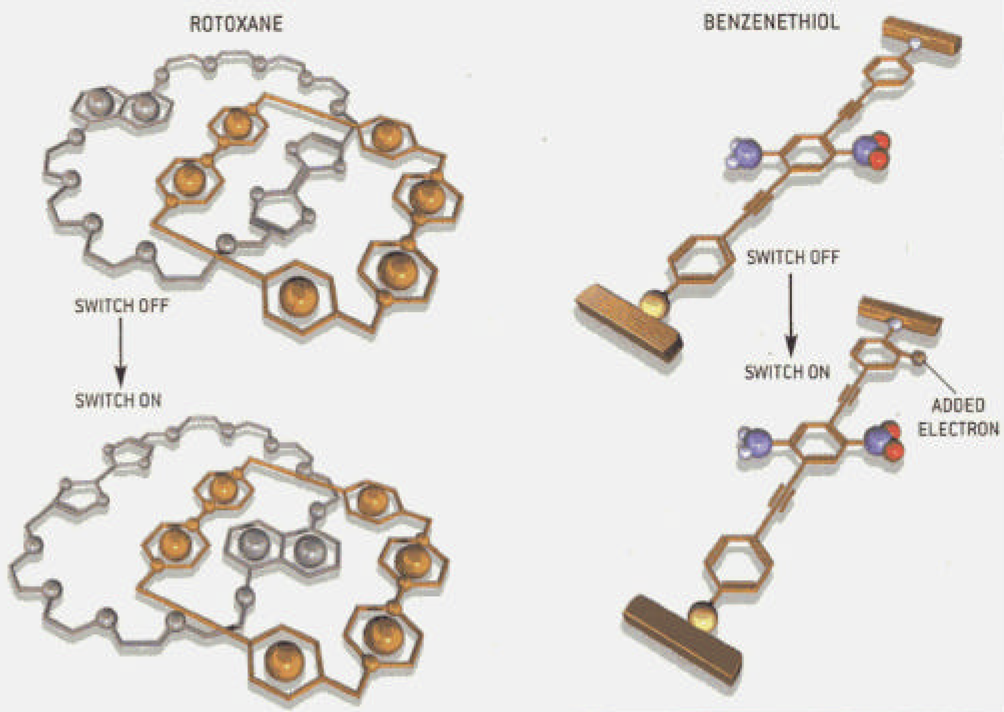
"There's plenty of room at the bottom" -- Richard Feynman, 1959.

Some Exotic Future Computing Technologies

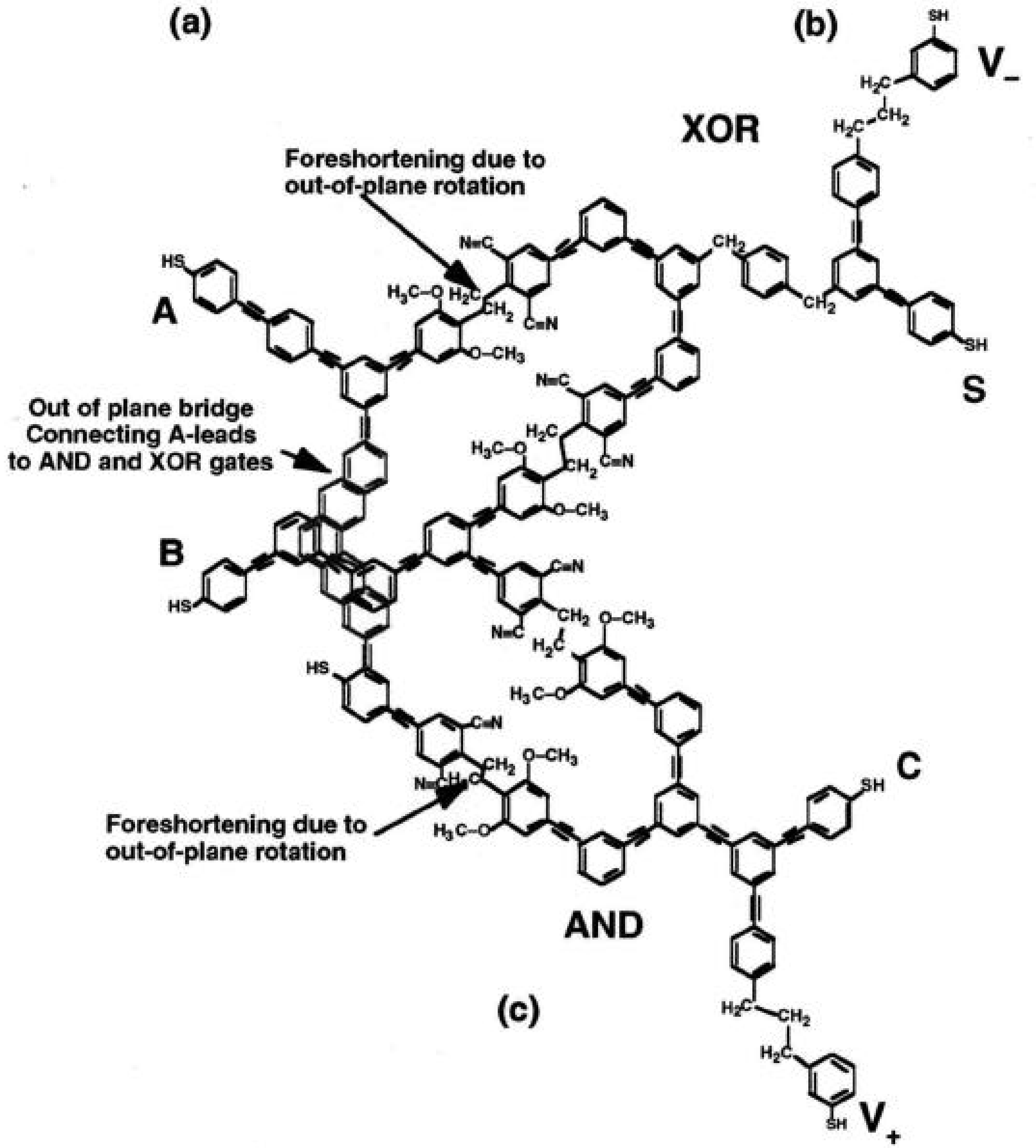
- Nanotubes
  - Nanotubes can be constructed to function as conductors and transistors.
- Molecular electronics
  - Arrays of organic molecules can be constructed to function as conductors and logic gates.
- DNA computing
  - Has been demonstrated for a simple application.
- Quantum computing
  - Potentially very powerful, if it can be realized.

Molecular Transistors
[Scientific American, Sept 2001]

MOLECULAR TRANSISTORS could be the building blocks of electronics on the nanometer scale. Each of the two molecules shown here conducts electricity like a tiny wire once a chemical reaction—oxidation reduction—alters its atomic configuration and switches it on. In the diagram, each stick represents a chemical bond; each intersection of two sticks represents a carbon atom; and each ball represents an atom other than carbon.



Molecular Add Circuit
[Ellenbogen, MITRE]



Conclusion

- There is no shortage of valuable scientific applications for future high-end computers.
- There is no shortage of ideas for future high-end system designs.
- There is no shortage of ideas for future high-end hardware technology.

Thus progress in high-end computing will likely continue for the foreseeable future.